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Consequences of the order of the limit of infinite spacetime volume and the sum over topological sectors for CP violation in the strong interactions

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ABSTRACT

We derive correlation functions for massive fermions with a complex mass in the presence of a general vacuum angle. For this purpose, we first build the Green's functions in the one-instanton background and then sum over the configurations of background instantons. The quantization of topological sectors follows for saddle points of finite Euclidean action in an infinite spacetime volume and the fluctuations about these. For the resulting correlation functions, we therefore take the infinite-volume limit before summing over topological sectors. In contrast to the opposite order of limits, the chiral phases from the mass terms and from the instanton effects then are aligned so that, in absence of additional phases, these do not give rise to observables violating charge-parity symmetry. This result is confirmed when constraining the correlations at coincident points by using the index theorem instead of instanton calculus.

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1. Introduction

The theoretical formulation of the strong interactions in general allows for a Lagrangian term

$$1/(16\pi^2)\theta\,\mathrm{tr}\,F\widetilde{F} \qquad (1)$$

that is odd (i.e. it changes sign) under charge-parity (CP) conjugation. Here, F is the gauge field strength tensor and $\widetilde{F}$ is its Hodge dual, with electric and magnetic components being interchanged. One may expect in general that this term also leads to phenomena that violate CP.

Conceivable in particular is a permanent electric dipole moment of the neutron [1,2], which, together with other potential indications of strong CP-violation, has not been observed to date. Since in first place, there is no reason to prefer $\theta = 0$ (or an integer multiple of π), it is therefore argued that the absence of such signals constitutes a shortcoming of the theory, referred to as the strong CP problem, and that it requires an extension of the Standard Model of particle physics. Theoretical research in this direction is extensive, and there is a number of experiments hunting for a proposed particle, the axion, that arises in many of these extensions [3].

From the Lagrangian, the action follows by integration over the spacetime. Since the CP-odd term (1) turns out to be a total derivative, the corresponding contribution to the action is determined by the boundary conditions on the gauge fields. Taking these to be vanishing physical fields, i.e. pure gauge configurations, at the boundary of spacetime, the integrals over the CP-odd term yield θ times integer values Δn—to be referred to as winding number or topological charge—corresponding to so-called homotopy classes that categorize maps of a three-dimensional sphere onto itself, where maps in different classes cannot be continuously transformed into one another [4,5].

This topological quantization is of central relevance when evaluating the effects from the term (1). One implication is, for example, that if the predictions of the theory depend on θ, they must be periodic in this parameter. This is because in the quantized theory, the action enters the path integral as a phase. The theory is therefore invariant under replacements $\theta \to \theta + 2\pi n$, where $n \in \mathbb{Z}$. Therefore, θ is sometimes referred to as the vacuum angle. Further, topological quantization implies that observables are to be calculated from an interference of amplitudes from different topological sectors, i.e. from path integrals for a given Δn or homotopy class, in the infinite spacetime.

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To state a principle leading to vanishing physical boundary conditions and therefore to topological quantization, we note that the nonvanishing contributions to the Euclidean path integral arise from saddle points of finite action and fluctuations around these. Saddle points correspond to solutions to the Euclidean equations of motion, and for these to exist in the infinite spacetime volume, the physical boundary conditions must vanish. As a consequence, the path integrals for the different topological sectors must then be evaluated in infinite spacetime volumes first. Otherwise, there would be no reason to assume topological quantization. In a second step, amplitudes from the different topological sectors are then to be interfered.

On the other hand, for boundary conditions imposed on finite spacetime volumes, saddle points and solutions to the equations of motion exist for nonvanishing physical fields at the boundaries as well. Moreover, the ground state configuration, that should determine the boundary conditions on finite spacetime volumes, is neither a field eigenstate nor a pure gauge configuration, i.e. it does not correspond to vanishing physical fields. In contrast, the Euclidean path integral in infinite volumes automatically projects the pure gauge field eigenstates on the corresponding accessible ground states. Nonetheless, if there were a principle that would lead to topological quantization for boundary conditions imposed on some finite surface, one could interfere the topological sectors prior to taking the spacetime volume to infinity.

Here, we show that the material consequence of the order of the limits is as follows: When taking the spacetime volume to infinity before interfering the topological sectors, CP-violating phenomena are absent in the strong interactions without extending the theory or setting the CP-odd term to zero. On the other hand, interfering the topological sectors before taking the spacetime volume to infinity, one concludes that correlation functions exhibit CP-violation that cannot be removed by field redefinitions [6].

The question of whether there is CP violation in general in the strong interactions of massive quarks should not be a matter of choice but be a prediction of the theory. Appended to this letter is therefore extensive supplementary material that addresses many aspects of the limiting procedure as well as pertaining matters such as the principle of cluster decomposition.

Technically, we arrive at our conclusions by computing the correlation functions for massive fermions, where we keep θ as well as the phase of the determinant of the matrix of quark masses general. As one of the methods, we use the leading approximation to a dilute gas of instantons so that the spacetime-dependence of the correlations can be recovered. As an alternative route, using arguments based on factorization properties of path integrals and the Atiyah-Singer index theorem [7], we confirm that the coincident limit of the fermion correlations does not exhibit CP violation, provided the interference of the topological sectors takes place among infinite spacetime volumes. Hence, the main results of this work hold beyond the perturbative expansion about instanton configurations. They crucially rely on how topological quantization emerges in spacetimes of infinite volume and the order in which the pertaining limits are carried out.

2. Topological charge, massive quarks, and charge-parity violation

In electrodynamics, the topological term (1) is immaterial because its volume integral can be traded for a surface integral over the boundaries of spacetime where it can be shown that finite action configurations have fields decaying fast enough such that the integral vanishes. This is not true for the strong interactions, where, due to the self-interactions, extended field configurations with finite action, so-called instantons, exist while the surface term

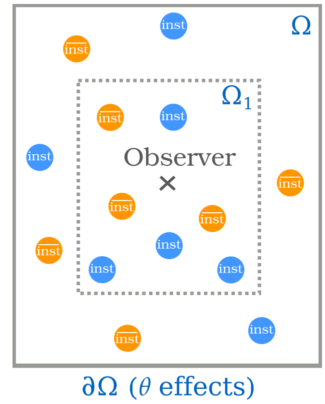

Fig. 1. For local quantum field theory, an observer is expected to be only sensitive to fluctuations in a local subvolume $\Omega_1 \subset \Omega$ in the limit of an infinite volume of the spacetime Ω. The θ-parameter influences the conditions at the boundary $\partial\Omega$. It can be shown that these do not affect the fluctuations in the subvolume. Fluctuations corresponding to instantons and anti-instantons are depicted as blue and orange circles, respectively.

no longer vanishes [8]. For this reason, it has been proposed that values of $\theta \neq \pi m$ $(m \in \mathbb{Z})$ may imply CP-violation [1,2,4,5].

While the topological term is local in the first place, and while in singular gauges the topological flux can be constrained to infinitesimal surfaces about the centres of the instantons [9], Eq. (1) is nonetheless equivalent to a surface term at the boundary of the spacetime at infinite distance. It is therefore an essential point whether it affects local observables in quantum field theory. The standard view is that this is the case because of a change in the local vacuum structure imposed by the boundary term. On the other hand, as illustrated in Fig. 1, one can approximate observables by including the fluctuations in a subvolume of the spacetime with all possible boundary conditions on its surface. One may expect—and it is possible to show this—that the theory in the subvolume is then independent of the boundary conditions in the infinite distance so that these have no material impact.

Intricately related with the topological term are CP-odd contributions to quark masses that can be expressed through $\bar{\psi}_j m_j \mathrm{e}^{\mathrm{i}\alpha_j\gamma^5}\psi_j$ where $j = 1, \ldots, N_f$ and N_f is the number of quark flavours. The quark fields are denoted by the spinors ψ_j, γ^5 is a matrix in spinor space and the phases α_j are CP-odd. The phases α_j can in principle be removed by redefinitions of the quark fields. However, since the so-called chiral symmetry of the quark fields is anomalous [10,11], the quark phases are tied to the vacuum-angle θ. In particular, $\bar{\theta} = \theta + \bar{\alpha}$, where $\bar{\alpha} = \sum_{j=1}^{N_f}\alpha_j$, is a phase that remains invariant under field redefinitions.

In order to calculate the most important CP-violating effects from the topological term, one derives effective fermion interactions caused by the instantons as Lagrangian terms of the form [6,12,13]

$$-\Gamma_{N_f}\mathrm{e}^{\mathrm{i}\xi}\prod_{j=1}^{N_f}(\bar{\psi}_j P_{\mathrm{L}}\psi_j) - \Gamma_{N_f}\mathrm{e}^{-\mathrm{i}\xi}\prod_{j=1}^{N_f}(\bar{\psi}_j P_{\mathrm{R}}\psi_j)\,, \tag{2}$$

where Γ_{N_f} is a coefficient and the left and right chiral projectors are $P_{\mathrm{L,R}} = (1 \mp \gamma^5)/2$.

The interaction (2) implies that there is no chiral symmetry with an overall U(1) phase. In the effective chiral Lagrangian for low energies, where quantum chromodynamics (QCD) confines, there thus is the corresponding term

$$|\lambda|\mathrm{e}^{-\mathrm{i}\xi} f_\pi^4 \det U + |\lambda|\mathrm{e}^{\mathrm{i}\xi} f_\pi^4 \det U^\dagger\,, \tag{3}$$

where f_π is the pion decay constant, U is a field of the form of a unitary matrix describing the mesons and λ is a coefficient within the effective theory.

The aforementioned invariance of $\bar{\theta}$ under field redefinitions leaves two possibilities for the phase ξ compatible with the chiral anomaly (assuming that ξ is a function of α and θ, and that the effective action is periodic in these parameters):

- $\xi = \theta$, i.e. in general misaligned with mass terms such that there is CP violation,
- $\xi = -\bar{\alpha}$, i.e. aligned with mass terms such that there is no CP violation.

The restriction to the above choices can be understood in terms of a spurious chiral symmetry under which θ transforms or simply by demanding that the relative phases between the interactions of Eq. (2) and the tree-level mass terms remain invariant under field redefinitions. Based on the topological quantization of the path integral and the ensuing order of limits, we derive here the effective operator (2) and show that the second possibility, $\xi = -\bar{\alpha}$, is the one that is realized what implies that there is no CP violation in the strong interactions.

When relating these remarks to the literature, we note that the possibility $\xi = \theta$ is implied in most of the papers without dismissing $\xi = -\bar{\alpha}$. The early papers, as well as literature following these, on phenomenological CP violation in the strong interactions make use of the freedom of chiral field redefinitions in order to set $\theta = 0$ and attribute the CP-odd phases to the quark masses [1,2]. In the context of the present discussion, this corresponds to setting $\xi = \theta = 0$ while $\bar{\alpha} \neq 0$ in general. The case of $\xi = -\bar{\alpha}$ is apparently not pursued. Also more recent discussions of the coefficients of the operator (3), e.g. Ref. [14], do not mull over this latter possibility.

Reference [6] appears to contain the only direct calculation leading to $\xi = \theta$, making use of the dilute instanton gas approximation. As we point out in the present work, this conclusion relies on computing the interference among topological sectors in finite spacetime volumes and taking these to infinity afterwards. Reversing this order of limits, as it is indicated when topological quantization emerges from the requirement of finite saddles in the action in infinite spacetimes, we show in the present work that one is led to conclude that $\xi = -\bar{\alpha}$ instead.

The interactions (3) are directly related to CP-violating observables such as a permanent electric dipole moment of the neutron or the decays $\eta' \to 2\pi$ (Section S3.6). For $\xi = \theta$, one recovers the standard results [1,2,15], while for $\xi = -\bar{\alpha}$, these signals vanish.

3. Fermion correlations in a dilute instanton gas

In this section we show that $\xi = -\bar{\alpha}$ by computing the quark correlation function in the approximation of a dilute instanton gas. In order to simplify notation, we set $N_f = 1$ and drop the index for the quark flavour. One should keep in mind that for a single quark flavour, the instanton effects amount to an addition to the quark mass. However, the generalization to the cases with $N_f > 1$ relevant for the potentially CP-violating phenomenology follows along the lines of the simplified analysis.

To compute the correlation function, we use the following Green's function in the background of n instantons (with topological charge $+1$) and $\bar{n}$ anti-instantons (with topological charge -1) located at $x_{0,\nu}$, $x_{0,\bar{\nu}}$ respectively:

$$\mathrm{i}S_{n,\bar{n}}(x,x') \approx \mathrm{i}S_{0\mathrm{inst}}(x,x') + \sum_{\bar{\nu}=1}^{\bar{n}} \frac{\varphi_{0\mathrm{L}}(x-x_{0,\bar{\nu}})\varphi^\dagger_{0\mathrm{L}}(x'-x_{0,\bar{\nu}})}{m\mathrm{e}^{-\mathrm{i}\alpha}} + \sum_{\nu=1}^{n} \frac{\varphi_{0\mathrm{R}}(x-x_{0,\nu})\varphi^\dagger_{0\mathrm{R}}(x'-x_{0,\nu})}{m\mathrm{e}^{\mathrm{i}\alpha}}. \quad (4)$$

This approximation is valid for a dilute instanton gas and quark masses such that m is small compared to $1/\varrho$, where ϱ is the radius of the instantons (which is not fixed). The spinors $\varphi_{0\mathrm{L,R}}$ are the analytic continuation of the zero modes of the Euclidean Dirac operator in the (anti-)instanton background, that determines the equation of motion for the quark fields, in the massless limit, and

$$\mathrm{i}S_{0\mathrm{inst}}(x,x') = (-\gamma^\mu\partial_\mu + \mathrm{i}m\mathrm{e}^{-\mathrm{i}\alpha\gamma^5}) \int \frac{\mathrm{d}^4p}{(2\pi)^4} \mathrm{e}^{-\mathrm{i}p(x-x')} \frac{1}{p^2 - m^2 + \mathrm{i}\epsilon} \quad (5)$$

is the solution in a background without instantons and is approximately valid at large distances from the individual locations, i.e. in between the instantons and anti-instantons.

Further, we readily assume here Minkowski metric. The approximation (4) has been used e.g. in Ref. [16] for $\alpha = 0$. The generalization to $\alpha \neq 0$ may appear obvious but there are some complications when transforming the spectrum of the Dirac operator from Euclidean to Minkowski spacetime. Yet, these can be addressed in detail thus confirming the form of the propagator (4) (Section S2). Note that the Green's function (4) is independent of θ because the topological term has not yet entered the derivation. However, it needs to be taken into account when summing configurations corresponding to different homotopy classes in the path-integral expression for the correlation function.

Here, we use the saddle point approximation to the path integral, where we sum over all instanton and anti-instanton numbers n and $\bar{n}$ and integrate over the locations of instantons and anti-instantons as well as over the remaining collective coordinates such as the radii ϱ and gauge orientations (which are independent for each instanton and anti-instanton).

The question of whether $\xi = -\alpha$ or $\xi = \theta$ is decided by the treatment of the summation over n and $\bar{n}$ in conjunction with how boundary conditions are imposed on the path integral. Let Ω denote the volume of spacetime and first consider Minkowski space such that Ω is infinite. The case of finite Ω is discussed below. Boundary conditions on the path integral are fixed by requiring that the physical gauge fields (as well as all other fields) vanish on the boundary of $\partial\Omega$, such that the action takes finite values at its saddle points [17] (Section S3.2). For the gauge field, this leaves open the possibility of pure gauge configurations.

These remarks apply to field configurations that are regular in Ω. In calculations aiming for interactions beyond the dilute instanton gas [16,18], it can be advantageous to use the singular gauge [9] so that one avoids working with integrands that are not manifestly square integrable. The price to pay for this is that there are singularities at the centres of the instantons or their approximate deformations. While spacetime needs to be punctured at these singularities, there are no apparent problems in constructing saddle point approximations to the path integral. Since the singular contributions at the centres of the instantons are pure gauges, the topological flux through an infinitesimal ball around such a point is again quantized. Then, for infinite Ω the fields still must vanish on $\partial\Omega$ but there is no topological flux through $\partial\Omega$, in contrast to the regular gauge. In effect, topological quantization results from the requirement of finite saddle point configurations in infinite spacetime volumes also in the singular gauge. In contrast, when restricting spacetime to finite Ω, there are finite saddle points for arbitrary nonsingular boundary conditions on $\partial\Omega$. Hence, some different principle would again be necessary to impose topological quantization for finite boundaries.

Both $\partial\Omega$ and $\mathrm{SU}(2) \subset \mathrm{SU}(3)$ (i.e. the subgroup of the group of gauge symmetries of the strong interactions) are homeomorphic to the three-dimensional sphere S^3 such that the gauge configurations fall into classes according to the third homotopy group. These characterize the number of times Δn a three-dimensional hypersurface can be wrapped around S^3. In the context of strong interactions, the class of configurations with boundary conditions corresponding to a certain Δn are sometimes referred to as a topological sector.

This property is of relevance for the present case because in the saddle point approximation $\Delta n = n - \bar{n}$. Furthermore, it is possible to define vacuum states $|n_{\rm CS}\rangle$ with a certain integer Chern–Simons number $n_{\rm CS}$. Taking the matrix element characterized by $\langle m_{\rm CS}|$ and $|n_{\rm CS}\rangle$ corresponds to fixing the topological sector $\Delta n = m_{\rm CS} - n_{\rm CS}$. We also note that the states $|n_{\rm CS}\rangle$ are not gauge invariant as the Chern–Simons number (defined on a spatial hypersurface) can change by all possible integer values through so-called large gauge transformations that are not continuously connected to the identity component. Thus, the true vacuum state should be constructed as a superposition of all Chern–Simons numbers of equal weight, but there may be relative phases proportional to $n_{\rm CS}$. These phases are effectively equivalent with the topological term in the action when calculating expectation values using the path integral approach. Since different topological sectors are distinguished by the boundary conditions which are taken at infinity, contributions to the path integral within a fixed topological sector must be evaluated for infinite spacetime volumes Ω. Note that this reasoning also applies to spacetime manifolds with compact spatial hypersurfaces yet with an infinite time direction. The possibility of restricting the integration to finite subvolumes of spacetime is discussed below.

The fermion correlator should therefore be evaluated as

$$\begin{aligned}
&\langle\psi(x)\bar{\psi}(x')\rangle \\
&= \lim_{\substack{N\to\infty\\ N\in\mathbb{N}}} \lim_{\Omega\to\infty} \frac{1}{Z(N,\Omega)} \sum_{\substack{m_{\rm CS},n_{\rm CS}\\ |m_{\rm CS}-n_{\rm CS}|\le N}} \langle m_{\rm CS}|\psi(x)\bar{\psi}(x')|n_{\rm CS}\rangle \\
&= \lim_{\substack{N\to\infty\\ N\in\mathbb{N}}} \lim_{\Omega\to\infty} \frac{\sum_{\Delta n=-N}^{N}\sum_n \langle n_{\rm CS}+\Delta n|\psi(x)\bar{\psi}(x')|n_{\rm CS}\rangle}{\sum_{\Delta n=-N}^{N} Z_{\Delta n}(\Omega)} \\
&= \lim_{\substack{N\to\infty\\ N\in\mathbb{N}}} \lim_{\Omega\to\infty} \frac{\sum\limits_{\Delta n=-N}^{N} \langle\psi(x)\bar{\psi}(x')\rangle_{\Delta n}}{\sum_{\Delta n=-N}^{N} Z_{\Delta n}(\Omega)}\,, \qquad (6)
\end{aligned}$$

where $Z(N,\Omega)$ and $Z_{\Delta n}(\Omega)$ are the partition function summed for all sectors $|\Delta n| \le N$ and that for a single topological sector, respectively. The dependence on N and Ω needs to be kept before taking these parameters to infinity. The order of the two limits in the last expression determines whether one arrives at $\xi = -\alpha$ or $\xi = \theta$, as we discuss next.

Now we need to consider the fermion correlator in a fixed topological sector. For a single flavour one has:

$$\begin{aligned}
&\langle\psi(x)\bar{\psi}(x')\rangle_{\Delta n} \\
&= \sum_{\substack{\bar{n},n\ge 0\\ n-\bar{n}=\Delta n}} \frac{1}{\bar{n}!n!}\Big[\bar{h}(x,x')\Big(\frac{\bar{n}}{m\mathrm{e}^{-\mathrm{i}\alpha}}P_{\rm L} + \frac{n}{m\mathrm{e}^{\mathrm{i}\alpha}}P_{\rm R}\Big)\Omega^{\bar{n}+n-1} \\
&\quad + \mathrm{i}S_{0\rm inst}(x,x')\Omega^{\bar{n}+n}\Big] \times (-\mathrm{i}\kappa)^{\bar{n}+n}\mathrm{e}^{\mathrm{i}\Delta n(\alpha+\theta)} \\
&= \Big[\Big(\mathrm{e}^{\mathrm{i}\alpha}I_{\Delta n+1}(2\mathrm{i}\kappa\Omega)P_{\rm L} + \mathrm{e}^{-\mathrm{i}\alpha}I_{\Delta n-1}(2\mathrm{i}\kappa\Omega)P_{\rm R}\Big)\frac{\mathrm{i}\kappa}{m}\bar{h}(x,x') \\
&\quad + I_{\Delta n}(2\mathrm{i}\kappa\Omega)\mathrm{i}S_{0\rm inst}(x,x')\Big] \times (-1)^{\Delta n}\mathrm{e}^{\mathrm{i}\Delta n(\alpha+\theta)}\,. \qquad (7)
\end{aligned}$$

In this expression, $\bar{h}(x,x')$ is a spinor correlation that remains after the integration of the instanton and anti-instanton locations as well as the collective coordinates and κ includes the exponential suppression of the instanton action—as these correspond to tunnelling processes—as well as extra factors that appear when evaluating the path integral to one-loop accuracy (Section S3.1). Finally, $I_\alpha(x)$ is the modified Bessel function of order α.

It is clear that the dilute instanton gas approximation does not apply directly to QCD. Rather, one could think of a nonabelian gauge theory whose particle content is made up such that the running coupling remains perturbative in the infrared and there is asymptotic freedom in the ultraviolet. In such a model, the scale invariance is broken radiatively such that there is no dilatational modulus and instead a preferred instanton size. That the symmetry properties with respect to CP of such a theory in principle also apply to QCD should therefore be taken as a more or less plausible assumption. In Section 4, we thus also present a derivation of the coincident fermion correlations that does not rely on the dilute instanton gas approximation.

The volume factors Ω in Eq. (7) are resulting here from the integration of the instanton locations over the entire spacetime. These appear in the same form even when taking these volumes to be finite for a given topological sector before interfering between these [6,16,18]. It is then understood that Ω, which is taken to infinity after interfering the topological sectors, is much larger than other scales that appear in the dilute instanton gas. This includes the mean separation between instantons and anti-instantons as well the typical size of these. In fact, restricting Ω to small volumes given by some physical length scale so that these only contain few instantons would substantially alter the results of e.g. Refs. [6,16,18] that do not impose such truncations on the path integral. The fact that the instanton locations are to be integrated over the entire spacetime is tied to translational invariance and mathematically derives from trading the translational moduli for collective coordinates [13,19]. It can also be seen in analogy with the calculation of the partition function for a classical ideal gas, where the individual positions of the particles are integrated over the entire configuration space. Beyond the dilute gas approximation, the spacetime integrations should be modified to account for the overlap of instantons and anti-instantons due to their finite size while yet, the individual locations are still to be integrated over infinite volumes [16]. For a theory to which the dilute gas approximation applies, omitting such corrections only amounts to a controllable error.

From Eq. (7), we see explicitly that in a fixed topological sector and large spacetime volumes Ω, the modulus of the coefficients of the left and right chiral contributions tends to the same value. In particular, for $x \to \infty$ and $|\arg(x)| < \pi/2$, $I_\alpha(x) \sim \exp(x)/\sqrt{2\pi x}$, i.e. these functions become independent of their index. As a consequence, for $\Omega \to \infty$, all topological sectors contribute in precisely the same way. Moreover, the chiral phases from the mass term contained in $S_{0\rm inst}$ (see Eq. (5)) and those induced by instanton effects are aligned, as a consequence of these phases (that originate from the fermion determinants and the topological term) being fixed by the boundary conditions on the topological sector Δn as we illustrate in Fig. 2. When normalizing by the partition function, the modified Bessel functions as well as the phase proportional to Δn cancel and we obtain

$$\langle\psi(x)\bar{\psi}(x')\rangle = \mathrm{i}S_{0\rm inst}(x,x') + \frac{\mathrm{i}\kappa}{m}\bar{h}(x,x')\mathrm{e}^{-\mathrm{i}\alpha\gamma^5}\,, \qquad (8)$$

such that the explicit phase can be identified with $\xi = -\alpha$. In contrast, if we were turning around the order of limits in Eq. (6), we would sum over two independent exponential series for n and $\bar{n}$ and find θ rather than $-\alpha$ in Eq. (8) so that $\xi = \theta$ (Section S3.3).

Taking the correct order of limits, i.e. $\Omega \to \infty$ before summing over topological sectors therefore explains the absence of CP violation in the strong interactions. This result can be generalized to an arbitrary number of fermion flavours (Section S3.4).

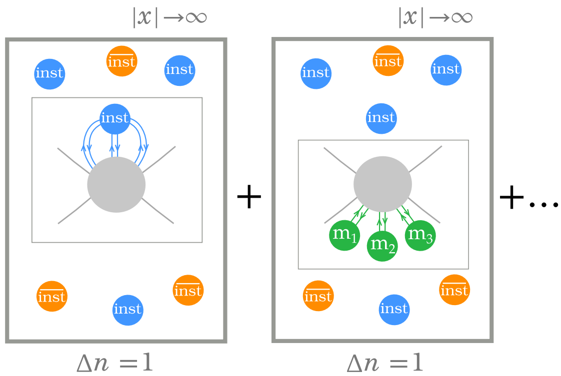

Fig. 2. Schematically shown are two contributions to a four-point correlation function in some multi-instanton background. The shaded blobs represent some subdiagram. On the left, there is a piece induced by a six-point fermion Green's function in the background of an instanton (corresponding to $\bar{h}$ in the two-point case). On the right, an interaction of the same chiral structure is induced by the fermion mass terms $m_{1,2,3}$ (corresponding to $\mathrm{i}S_{0\mathrm{inst}}$ in the two-point case). When integrating over the subvolumes indicated by the thin grey boxes only, the left piece would acquire a relatively misaligned phase $\theta+\alpha$ (α being here the sum of the quark mass phases) compared to the right piece because the phases come from the topological term and the fermion determinants. When instead correctly computing the path integral over the full spacetime volume (represented by the thick grey boundaries), the phase for both pieces is aligned and given by $\Delta n(\theta+\alpha)$. For infinite spacetime volumes, the interferences between the different sectors Δn moreover are immaterial.

4. Chiral correlations from the index theorem

In this section we provide an alternative derivation of the previous results without using instantons. The starting point are the factorization properties of the path integration when the full spacetime volume Ω is divided into subvolumes Ω_1 and Ω_2. Following standard textbook arguments used in the context of cluster decomposition [20], the fact that the topological charge Δn is a surface flux allows to write the partition function of the full spacetime volume $\Omega=\Omega_1\cup\Omega_2$ as

$$Z_{\Delta n}(\Omega)=\sum_{\Delta n_1=-\infty}^{\infty} Z_{\Delta n_1}(\Omega_1)Z_{\Delta n-\Delta n_1}(\Omega_2). \tag{9}$$

For convenience, in this section we work in Euclidean space, as this simplifies the tracking of the complex phases. First we can extract the θ-dependent phase, $Z_{\Delta n}(\Omega)\propto \mathrm{e}^{\mathrm{i}\Delta n\theta}$. Any additional complex phases can only come from the integration over fermionic fluctuations. To leading order in a loop expansion around saddle points, these integrations have the form of determinants of the Dirac operator in each saddle-point background. Here we make no approximation of the saddle points in terms of a dilute instanton gas.

Parity transformations relate pairs of eigenfunctions of the massive Dirac operator with mutually conjugate eigenvalues, except for those eigenfunctions that, being zero modes of the massless operator, have eigenvalues given by the complex fermion masses, resulting in opposite phases for right-handed and left-handed modes (Section S2.2). Hence the phase of the full determinant within a topological class characterized by Δn is determined by the difference between the number of right and left-handed zero modes of the massless Dirac operator, which according to the Atiyah-Singer index theorem coincides with Δn [7]. This gives a phase of $\mathrm{e}^{\mathrm{i}\Delta n\bar{\alpha}}$ for the product of all fermion determinants. As a consequence, we may write

$$Z_{\Delta n}(\Omega)=\mathrm{e}^{\mathrm{i}\Delta n\bar{\theta}}\tilde{g}_{\Delta n}(\Omega) \tag{10}$$

with real $\tilde{g}_{\Delta n}(\Omega)$. Equation (9) gives then the relations

$$\tilde{g}_{\Delta n}(\Omega_1+\Omega_2)=\sum_{\Delta n_1=-\infty}^{\infty}\tilde{g}_{\Delta n_1}(\Omega_1)\tilde{g}_{\Delta n-\Delta n_1}(\Omega_2). \tag{11}$$

Setting $\Omega_i=0$ above can be seen to imply that $\tilde{g}_{\Delta n}(0)=\delta_{\Delta n,0}$. We next note that parity transformations relate Δn with $-\Delta n$. As the $\tilde{g}_{\Delta n}$ are real and not sensitive to parity-violating effects from the complex fermion masses, one has $\tilde{g}_{-\Delta n}(\Omega)=\tilde{g}_{\Delta n}(\Omega)$. The former results motivate the Ansatz

$$\tilde{g}_{\Delta n}(\Omega)=\Omega^{|\Delta n|}f_{|\Delta n|}(\Omega^2),\quad f_{|\Delta n|}(0)\neq 0. \tag{12}$$

Remarkably, assuming analyticity in Ω (and as shown in Section S4), there is a unique solution which, upon substitution in Eq. (10), gives

$$Z_{\Delta n}(\Omega)=I_{\Delta n}(2\beta\Omega)\,\mathrm{e}^{\mathrm{i}\bar{\theta}\Delta n}, \tag{13}$$

where β depends on the parameters of the theory and is not determined at the present level of generality. This has the same form as the result for the partition function in the dilute gas approximation (Section S3.1).

Finally we note that since all dependence on the complex fermion masses is included in $\bar{\theta}$, β can only depend on the moduli of the complex fermion masses $\mathfrak{m}_j\equiv m_j\mathrm{e}^{\mathrm{i}\alpha_j}$: $\beta=\beta(\mathfrak{m}_j\mathfrak{m}_j^*)$. In order to obtain fermion correlators, it suffices to note that $\mathfrak{m}_j$ and $\mathfrak{m}_j^*$ can be seen as sources for integrated two-point functions. Within a fixed topological sector Δn, the volume averages of the fermionic correlators can be obtained as

$$\begin{aligned}\frac{1}{\Omega}\int \mathrm{d}^4x\,\langle\bar{\psi}_i P_{\mathrm{R}}\psi_i\rangle_{\Delta n}&=-\frac{1}{\Omega}\frac{\partial}{\partial\mathfrak{m}_i}Z_{\Delta n},\\ \frac{1}{\Omega}\int \mathrm{d}^4x\,\langle\bar{\psi}_i P_{\mathrm{L}}\psi_i\rangle_{\Delta n}&=-\frac{1}{\Omega}\frac{\partial}{\partial\mathfrak{m}_i^*}Z_{\Delta n}.\end{aligned} \tag{14}$$

Using Eq. (13) and summing over topological sectors after taking the limit $\Omega\to\infty$ as before gives correlators whose phases are aligned with the tree-level masses, leading to no CP violation:

$$\begin{aligned}\frac{1}{\Omega}\int \mathrm{d}^4x\,\langle\bar{\psi}_i P_{\mathrm{R}}\psi_i\rangle&=-2\mathfrak{m}_i^*\,\partial_{\mathfrak{m}_i\mathfrak{m}_i^*}\beta(\mathfrak{m}_k\mathfrak{m}_k^*),\\ \frac{1}{\Omega}\int \mathrm{d}^4x\,\langle\bar{\psi}_i P_{L}\psi_i\rangle&=-2\mathfrak{m}_i\,\partial_{\mathfrak{m}_i\mathfrak{m}_i^*}\beta(\mathfrak{m}_k\mathfrak{m}_k^*).\end{aligned} \tag{15}$$

By taking additional derivatives with respect to the masses $\mathfrak{m}_j$, $\mathfrak{m}_j^*$, the results can be extended to correlation functions involving more fermion fields.

5. Finite subvolumes, periodic boundary conditions and fixed topological sectors

To view this result from additional angles, we discuss what one would obtain for fixed topological sectors or for finite spacetime volumes. Taking the order of the limits as in Eq. (6), we have seen that the modified Bessel functions in Eq. (7) tend to a common limit. This can be seen as a consequence of $\Delta n/\Omega\to 0$. Taking $\Omega\to\infty$ before summing over different topological sectors may therefore be viewed to be equivalent with setting $\Delta n=0$ from the outset. This explains why taking limits as in Eq. (6) leads to the alignment between the various chiral phases. We note that a relevant example for finite Ω and fixed Δn is given by boundary conditions that are periodic in all four dimensions. This setup is mostly chosen in lattice simulations, where Δn freezes in the continuum limit.

In the approximation of the dilute instanton gas, it can be shown that fixing Δn in an infinite spacetime volume is compliant with the principle of cluster decomposition (Section S5.1). In finite spacetime volumes Ω, corrections to the asymptotic form of correlators required by the cluster decomposition principle then vanish, provided Ω is chosen large enough to meet a given precision (Section S5.2). This observation has also been made in Refs. [21,22] through different calculational methods. We therefore conclude that it is possible to describe the strong interactions in a fixed sector with finite Δn, provided Ω is large enough or infinite, and that there are no CP-violating effects in this theory.

With the above observation and working in a single topological sector with fixed Δn, we can evaluate the path integral in a finite subvolume $\Omega_1 \subset \Omega$ according to Fig. 1, no matter whether the full spacetime volume is finite or infinite. For such a setup, we need to sum or integrate over boundary conditions of a certain winding number Δn_1 (which is not necessarily integer because instantons can be located at the boundary). The full winding number Δn is however fixed by the boundary conditions on $\partial\Omega$. In particular, let $\Omega_2 = \Omega \setminus \Omega_1$ and Δn_2 be the winding number within Ω_2. Then, $\Delta n = \Delta n_1 + \Delta n_2$ remains fixed such that the total phase proportional to Δn separates just like in Eq. (7) and cancels within observables. One can then obtain expectation values from a path integration restricted to Ω_1 in which the θ dependence is absent, and once more the result (8) is recovered (Sections S5.1 and S5.2).

We emphasize that the fermion correlations evaluated according to Eq. (6) are compatible with the enhanced mass of the η'-meson compared to those mesons associated with spontaneously broken symmetries that are not anomalous (Section S3.6). This can be explained in more detail when observing that the chiral susceptibility evaluated in finite subvolumes of spacetime agrees with known results from the dilute instanton gas approximation and moreover when noting that even within a fixed topological sector, there is an η'-meson with enhanced mass (Section S5.4). Then one can also show that under reasonable assumptions the mass of the η' is proportional to the topological susceptibility of the pure gauge theory evaluated in finite subvolumes, which generalizes classic results derived for large numbers of colours in Refs. [23,24]. Finally, we note that arguments linking the topological susceptibility with CP violation [25] rely on assuming analyticity in θ of the partition function for the full volume, which does not apply when the infinite volume limit is taken before summing over the topological sectors (Sections S3.6 and S5.4).

6. Conclusions

In this work, we have derived fermion correlations in instanton backgrounds, investigated the cases of finite and infinite spacetime volumes and checked the compliance with cluster decomposition. If there were a valid principle that would allow the limit of infinite spacetime volume to be taken after the summation over topological sectors, we would recover CP-violating correlations proportional to the rephasing-invariant parameter $\bar{\theta}$. However, based on the reasoning that the quantization of the topological sectors comes from the fact that the path integral receives its nonvanishing contributions from saddle points of finite action and fluctuations about these, boundary conditions in Euclidean space should be imposed at infinity before the summation over topological sectors. The conclusion then is that the theory of strong interactions with massive fermions does not predict CP-violating phenomena, irrespective of the value of $\bar{\theta}$.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary material

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.physletb.2021.136616. The references in this Letter to Sections starting with 'S' refer to that material.

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